

1.3 DETERMINANT EVALUATION

We observe that even in the partial pivoting method we get matrices

$M^{(k)}, M^{(k-1)}, \dots, M^{(1)}$ such that

$M^{(k)} M^{(k-1)} \dots M^{(1)} A$ is upper triangular
and
therefore

$\det M^{(k)} \det M^{(k-1)} \dots \det M^{(1)} \det A =$ Product of the diagonal entries in the final upper triangular matrix.

Now $\det M^{(i)} = 1$ if it refers to the process of nullifying entries below the diagonal to zero; and

$\det M^{(i)} = -1$ if it refers to a row interchange necessary for a partial pivoting.

Therefore $\det M^{(k)} \dots \det M^{(1)} = (-1)^m$ where m is the number of row inverses effected in the reduction.

Therefore $\det A = (-1)^m$ product of the diagonal entries in the final upper triangular matrix.

In our example 1 above, we had $M^{(1)}, M^{(2)}, M^{(3)}, M^{(4)}$ of which $M^{(1)}$ and $M^{(3)}$ referred to row interchanges. Thus therefore there were two row interchanges and hence

$$\det A = (-1)^2 (2) \left(\frac{5}{2}\right) \left(\frac{9}{5}\right) = 9.$$

In example 2 also we had $M^{(1)}, M^{(3)}$ as row interchange matrices and therefore $\det A = (-1)^2 (0.215512) (0.361282) (0.188856) = 0.013608$

LU decomposition:

Notice that the M matrices corresponding to row interchanges are no longer lower triangular. (See $M^{(1)}$ & $M^{(3)}$ in the two examples.) Thus,

$$M^{(k)} M^{(k-1)} \dots M^{(1)}$$

is not a lower triangular matrix in general and hence using partial pivoting we cannot get LU decomposition in general.

1.4 GAUSS JORDAN METHOD

In this method we continue the partial pivoting method further to reduce, using Elementary Row Operations, the diagonal entries where the nonzero pivots are located to 1 and all other entries in the columns containing nonzero pivots to zero. The resulting matrix is called the Row Reduced Echelon (RRE) form of the given matrix, and is denoted by A_R . These Elementary Row Transformations correspondingly reduce the vector y to a form which we denote by y_R . This is the same as saying that the augmented matrix A_{aug} is reduced to the matrix $(A_R|y_R)$

Remark:

In case in the reduction process at some stage if we get $a_{rr} = a_{r+1r} = \dots = a_{r+nr} = 0$, then even partial pivoting does not bring any nonzero entry to r^{th} diagonal because there is no nonzero entry available. In such a case A is singular matrix and we proceed to the RRE form to get the general solution of the system. As observed earlier, in the case A is nonsingular, Gauss-Jordan Method leads to $A_R = I_n$ and the product of corresponding $M^{(i)}$ gives us A^{-1} .

1.5 L U DECOMPOSITIONS

We shall now consider the LU decomposition of matrices. Suppose A is an $n \times n$ matrix. If L and U are lower and upper triangular $n \times n$ matrices respectively such that $A = LU$, we say that this is a LU decomposition of A . Note that LU decomposition is not unique. For example if $A = LU$ is a decomposition then $A = L_\alpha U_\alpha$ is also a LU decomposition where $\alpha \neq 0$ is any scalar and $L_\alpha = \alpha L$ and $U_\alpha = 1/\alpha U$.

Suppose we have a LU decomposition $A = LU$. Then, the system, $Ax = y$, can be solved as follows:

$$\text{Set } Ux = z \quad \dots\dots\dots (1)$$

Then the system $Ax = y$ can be written as,

$$LUx = y,$$

i.e.,

$$Lz = y \quad \dots\dots\dots(2)$$

Now (2) is a triangular system – infact lower triangular and hence we can solve it by forward substitution to get z .

Substituting this z in (1) we get an upper triangular system for x and this can be solved by back substitution.

Further if $A = LU$ is a LU decomposition then, $\det. A$ can be calculated as
 $\det. A = \det. L \cdot \det. U$
 $= l_{11} l_{22} \dots l_{nn} u_{11} u_{22} \dots u_{nn}$

where l_{ii} are the diagonal entries of L , and u_{ii} are the diagonal entries of U .

Also A^{-1} can be obtained from an LU decomposition as $A^{-1} = U^{-1} L^{-1}$.

Thus an LU decomposition helps to break a given system into Triangular systems; to find the determinant of a given matrix; and to find the inverse of a given matrix.

We shall now give methods to find LU decomposition of a matrix. Basically, we shall be considering three cases. First, we shall consider the decomposition of a Tridiagonal matrix; secondly the Doolittles's method for a general matrix, and thirdly the Cholesky's method for a symmetric matrix.

I. TRIDIAGONAL MATRIX

Let

$$A = \begin{pmatrix} b_1 & a_2 & 0 & 0 & \dots & 0 \\ c_1 & b_2 & a_3 & 0 & \dots & 0 \\ 0 & c_2 & b_3 & a_4 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & c_{n-2} & b_{n-1} & a_n \\ 0 & \dots & \dots & 0 & c_{n-1} & b_n \end{pmatrix}$$

be an $n \times n$ tridiagonal matrix. We seek a LU decomposition for this. First we shall give some preliminaries.

Let δ_i denote the determinant of the i^{th} principal minor of A

$$\delta_i = \begin{vmatrix} b_1 & a_2 & 0 & \dots & 0 \\ c_1 & b_2 & a_3 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & c_{i-2} & b_{i-1} & a_i \\ 0 & \dots & 0 & c_{i-1} & b_i \end{vmatrix}$$

Expanding by the last row we get,

$$\left. \begin{aligned} \delta_i &= b_i \delta_{i-1} - c_{i-1} a_i \delta_{i-2}; i = 2,3,4, \dots \\ \delta_1 &= b_1 \end{aligned} \right\} \dots\dots\dots(I)$$

We define $\delta_0 = 1$

From (I) assuming that δ_i are all nonzero we get

$$\frac{\delta_i}{\delta_{i-1}} = b_i - c_{i-1} a_i \frac{\delta_{i-2}}{\delta_{i-1}}$$

Setting $\frac{\delta_i}{\delta_{i-1}} = k_i$ this can be written as

$$b_i = k_i + c_{i-1} \frac{a_i}{k_{i-1}} \dots\dots\dots(II)$$

Now we seek a decomposition of the form $A = LU$ where,

$$L = \begin{pmatrix} 1 & 0 & \dots & \dots & \dots & 0 \\ w_1 & 1 & 0 & \dots & \dots & 0 \\ 0 & w_2 & 1 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \dots & w_{n-1} & 1 \end{pmatrix}; U = \begin{pmatrix} u_1 & \alpha_2 & 0 & \dots & 0 \\ 0 & u_2 & \alpha_3 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & u_{n-1} & \alpha_n \\ 0 & 0 & \dots & 0 & u_n \end{pmatrix}$$

i.e. we need the lower triangular and upper triangular parts also to be 'Tridiagonal' triangular.

Note that if $A = (a_{ij})$ then because A is Tridiagonal, a_{ij} is nonzero only when i and j differ by 1. i.e. only a_{i-1i} , a_{ii} , a_{ii+1} are nonzero. In fact,

$$\left. \begin{aligned} a_{i-1i} &= a_i \\ a_{ii} &= b_i \\ a_{i+1i} &= c_i \end{aligned} \right\} \dots\dots\dots (III)$$

In the case of L and U we have

$$\left. \begin{aligned} l_{i+1i} &= w_i \\ l_{ii} &= 1 \\ l_{ij} &= 0 \text{ if i) } j>i \text{ or ii) } j<i \text{ with } i-j \geq 2. \end{aligned} \right\} \dots\dots\dots (IV)$$

$$\left. \begin{aligned} u_{ii+1} &= \alpha_{i+1} \\ u_{ii} &= u_i \\ u_{ij} &= 0 \text{ if i) } i>j \text{ or ii) } i<j \text{ with } j-i \geq 2. \end{aligned} \right\} \dots\dots\dots (V)$$

Now $A = LU$ is what is needed.

Therefore,

$$a_{ij} = \sum_{k=1}^n l_{ik} u_{kj} \dots\dots\dots (VI)$$

Therefore

$$a_{i-1i} = \sum_{k=1}^n l_{i-1k} u_{ki}$$

Using (III), (IV) and (V) we get

$$a_i = l_{i-1i-1} u_{i-1i} = \alpha_i$$

Therefore

$$\alpha_i = a_i \dots\dots\dots (VII)$$

This straight away gives us the off diagonal entries of U .

From (VI) we also get

$$a_{ii} = \sum_{k=1}^n l_{ik} u_{ki}$$

$$= L_{i-1}U_{i-1} + L_iU_i$$

Therefore

$$b_i = w_{i-1}\alpha_i + u_i \quad \dots\dots\dots (VIII)$$

From (VI) we get further,

$$\begin{aligned} a_{i+1} &= \sum_{k=1}^n l_{i+1k} u_{ki} \\ &= l_{i+1i}u_i + l_{i+1i+1}u_{i+1} \end{aligned}$$

$$c_i = w_i u_i$$

Thus $c_i = w_i u_i \quad \dots\dots\dots (IX)$

Using (IX) in (VIII) we get (also using $\alpha_i = a_i$)

$$b_i = \frac{c_{i-1}a_i}{u_{i-1}} + u_i$$

Therefore

$$b_i = u_i + \frac{c_{i-1}a_i}{u_{i-1}} \quad \dots\dots\dots (X)$$

Comparing (X) with (II) we get

$$u_i = k_i = \frac{\delta_i}{\delta_{i-1}} \quad \dots\dots\dots (XI)$$

using this in (IX) we get

$$w_i = \frac{c_i}{u_i} = \frac{c_i \delta_{i-1}}{\delta_i} \quad \dots\dots\dots (XII)$$

From (VII) we get

$$\alpha_i = a_i \quad \dots\dots\dots (XIII)$$

(XI), (XII) and (XIII) completely determine the matrices L and U and hence we get the LU decomposition.

Note : We can apply this method only when δ_i are all nonzero. i.e. all the principal minors have nonzero determinant.

Example :

$$\text{Let } A = \begin{pmatrix} 2 & -2 & 0 & 0 & 0 \\ -2 & 1 & 1 & 0 & 0 \\ 0 & -2 & 5 & -2 & 0 \\ 0 & 0 & 9 & -3 & 1 \\ 0 & 0 & 0 & 3 & -1 \end{pmatrix}$$

Let us now find the LU decomposition as explained above.

We have

$$\begin{array}{l} b_1 = 2 \qquad b_2 = 1 \qquad b_3 = 5 \qquad b_4 = -3 \qquad b_5 = -1 \\ c_1 = -2 \qquad c_2 = -2 \qquad c_3 = 9 \qquad c_4 = 3 \\ a_2 = -2 \qquad a_3 = 1 \qquad a_4 = -2 \qquad a_5 = 1 \end{array}$$

We have

$$\begin{aligned} \delta_0 &= 1 \\ \delta_1 &= 2 \\ \delta_2 &= b_2 \delta_1 - a_2 c_1 \delta_0 = 2 - 4 = -2 \\ \delta_3 &= b_3 \delta_2 - a_3 c_2 \delta_1 = (-10) - (-2)(2) = -6 \\ \delta_4 &= b_4 \delta_3 - a_4 c_3 \delta_2 \\ &= (-3)(-6) - (-18)(-2) = -18 \\ \delta_5 &= b_5 \delta_4 - a_5 c_4 \delta_3 \\ &= (-1)(-18) - (3)(-6) \\ &= 36. \end{aligned}$$

Note $\delta_1, \delta_2, \delta_3, \delta_4, \delta_5$ are all nonzero. So we can apply the above method.

Therefore by (XI) we get

$$u_1 = \frac{\delta_1}{\delta_0} = 2; u_2 = \frac{\delta_2}{\delta_1} = \frac{-2}{2} = -1; u_3 = \frac{\delta_3}{\delta_2} = \frac{-6}{-2} = 3$$

$$u_4 = \frac{\delta_4}{\delta_3} = \frac{-18}{-6} = 3; \quad \text{and} \quad u_5 = \frac{\delta_5}{\delta_4} = \frac{36}{-18} = -2$$

From (XII) we get

$$w_1 = \frac{c_1}{u_1} = \frac{-2}{2} = -1$$

$$w_2 = \frac{c_2}{u_2} = \frac{-2}{-1} = 2$$

$$w_3 = \frac{c_3}{u_3} = \frac{9}{3} = 3$$

$$w_4 = \frac{c_4}{u_4} = \frac{3}{3} = 1$$

From (XIII) we get

$$\alpha_2 = a_2 = -2$$

$$\alpha_3 = a_3 = 1$$

$$\alpha_4 = a_4 = -2$$

$$\alpha_5 = a_5 = 1$$

Thus;

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 & 0 \\ 0 & 0 & 3 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix} ; \quad U = \begin{pmatrix} 2 & -2 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 3 & -2 & 0 \\ 0 & 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

In the above method we had made all the diagonal entries of L as 1. This will facilitate solving the triangular system $Lz = y$ (equation (2) on page 19). However by choosing these diagonals as 1 it may be that the u_i , the diagonal entries in U become small thus creating problems in back substitution for the system $Ux = z$ (equation (1) on page 19). In order to avoid this situation Wilkinson suggests that in any triangular decomposition choose the diagonal entries of L and U to be of the same magnitude. This can be achieved as follows:

We seek

$$A = LU$$

where

$$L = \begin{pmatrix} l_1 & & & & \\ w_2 & l_2 & & & \\ & & \ddots & & \\ \circ & & & & \\ & & & & w_{n-1}l_n \end{pmatrix}$$

$$U = \begin{pmatrix} u_1 & \alpha_2 & 0 & \dots & 0 \\ 0 & u_2 & \alpha_3 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & u_{n-1} & \alpha_n \\ 0 & 0 & \dots & 0 & u_n \end{pmatrix}$$

$$l_{ii} = l_i$$

Now $l_{i+1i} = w_i$

$$l_{ij} = 0 \quad \text{if i) } j > i \text{ or ii) } j < i \text{ with } i-j \geq 2$$

$$u_{ii} = u_i$$

$$u_{i+1i} = \alpha_{i+1}$$

$$u_{ij} = 0 \quad \text{if i) } i > j; \text{ or ii) } j > i \text{ with } j-i \geq 2$$

Now (VII), (VIII) and (IX) change as follows:

$$a_i = a_{i-1i} = \sum_{k=1}^n l_{i-1k} u_{ki} = l_{i-1i-1} u_{i-1i} = l_{i-1} \alpha_i$$

Therefore

$$a_i = l_{i-1} \alpha_i \quad \dots\dots\dots (VII')$$

$$b_i = a_{ii} = \sum_{k=1}^n l_{ik} u_{ki} = l_{ii-1} u_{i-1i} + l_{ii} u_{ii}$$

$$= w_{i-1} \alpha_i + l_i u_i$$

Therefore

$$b_i = w_{i-1} \alpha_i + l_i u_i \quad \dots\dots\dots (VIII')$$

$$c_i = a_{i+1i} = \sum_{k=1}^n l_{i+1k} u_{ki}$$

$$= l_{i+1i} u_{ii}$$

$$= w_i u_i$$

$$c_i = w_i u_i \quad \dots\dots\dots (IX')$$

From (VIII') we get using (VII') and (IX')

$$b_i = \frac{c_{i-1}}{u_{i-1}} \cdot \frac{a_i}{l_{i-1}} + l_i u_i$$

$$= \frac{a_i c_{i-1}}{l_{i-1} u_{i-1}} + l_i u_i$$

$$b_i = \frac{a_i c_{i-1}}{p_{i-1}} + p_i \quad \dots\dots\dots (X')$$

where

$$p_i = l_i u_i$$

Comparing (X') with (II) we get

$$p_i = k_i = \frac{\delta_i}{\delta_{i-1}}$$

Therefore

$$l_i u_i = \frac{\delta_i}{\delta_{i-1}}$$

we choose $l_i = \sqrt{\left| \frac{\delta_i}{\delta_{i-1}} \right|}$ (XIV)

$$u_i = \left(\text{sgn} \frac{\delta_i}{\delta_{i-1}} \right) \sqrt{\left| \frac{\delta_i}{\delta_{i-1}} \right|} \quad \text{..... (XV)}$$

Thus l_i and u_i have same magnitude. These then can be used to get w_i and α_i from (VII') and (IX'). We get finally,

$$l_i = \sqrt{\left| \frac{\delta_i}{\delta_{i-1}} \right|} \quad ; \quad u_i = \left(\text{sgn} \cdot \frac{\delta_i}{\delta_{i-1}} \right) \sqrt{\left| \frac{\delta_i}{\delta_{i-1}} \right|} \quad \text{..... (XI')}$$

$$w_i = \frac{c_i}{u_i} \quad \text{..... (XII')}$$

$$\alpha_i = \frac{a_i}{l_{i-1}} \quad \text{..... (XIII')}$$

These are the generalizations of formulae (XI), (XII) and (XIII).

Let us apply this to our example matrix (on page 23).

We get;

$$\delta_0 = 1 \quad \delta_1 = 2 \quad \delta_2 = -2 \quad \delta_3 = -6 \quad \delta_4 = -18 \quad \delta_5 =$$

$$b_1 = 2 \quad b_2 = 1 \quad b_3 = 5 \quad b_4 = -3 \quad b_5 = -1$$

$$c_1 = -2 \quad c_2 = -2 \quad c_3 = 9 \quad c_4 = 3$$

$$a_1 = -2 \quad a_3 = 1 \quad a_4 = -2 \quad a_5 = 1$$

$$\text{We get } \delta_1/\delta_0 = 2 ; \delta_2/\delta_1 = -1 ; \delta_3/\delta_2 = 3 ; \delta_4/\delta_3 = 3 ; \delta_5/\delta_4 = -2$$

Thus from (XI') we get

$$\left. \begin{array}{l} l_1 = \sqrt{2} \quad u_1 = \sqrt{2} \\ l_2 = 1 \quad u_2 = -1 \\ l_3 = \sqrt{3} \quad u_3 = \sqrt{3} \\ l_4 = \sqrt{3} \quad u_4 = \sqrt{3} \end{array} \right\}$$

From (XII') we get

$$w_1 = \frac{C_1}{u_1} = \frac{-2}{\sqrt{2}} = -\sqrt{2} \quad ; \quad w_2 = \frac{C_2}{u_2} = \frac{-2}{-1} = 2 \quad ;$$

$$w_3 = \frac{C_3}{u_3} = \frac{9}{\sqrt{3}} = 3\sqrt{3} \quad ; \quad w_4 = \frac{C_4}{u_4} = \frac{3}{\sqrt{3}} = \sqrt{3}$$

From (XIII') we get

$$\alpha_2 = \frac{a_2}{l_1} = \frac{-2}{\sqrt{2}} = -\sqrt{2} \quad ; \quad \alpha_3 = \frac{a_3}{l_2} = \frac{1}{1} = 1 \quad ;$$

$$\alpha_4 = \frac{a_4}{l_3} = \frac{-2}{\sqrt{3}}; \quad \alpha_5 = \frac{a_5}{l_4} = \frac{1}{\sqrt{3}}$$

Thus, we have LU decomposition,

$$A = \begin{pmatrix} 2 & -2 & 0 & 0 & 0 \\ -2 & 1 & 1 & 0 & 0 \\ 0 & -2 & 5 & -2 & 0 \\ 0 & 0 & 9 & -3 & 1 \\ 0 & 0 & 0 & 3 & -1 \end{pmatrix} = \underbrace{\begin{pmatrix} \sqrt{2} & 0 & 0 & 0 & 0 \\ -\sqrt{2} & 1 & 0 & 0 & 0 \\ 0 & 2 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 3\sqrt{3} & \sqrt{3} & 0 \\ 0 & 0 & 0 & \sqrt{3} & \sqrt{2} \end{pmatrix}}_L \underbrace{\begin{pmatrix} \sqrt{2} & -\sqrt{2} & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{3} & -\frac{2}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & \sqrt{3} & \frac{1}{\sqrt{3}} \\ 0 & 0 & 0 & 0 & -\sqrt{2} \end{pmatrix}}_U$$

in which the L and U have corresponding diagonal elements having the same magnitude.